

Claims

What is claimed is:

- 5 1. A method for calculating a moment of a tertiary protein structure comprising a plurality of residues, the method comprising the steps of:
 - calculating a centroid of residue centroids;
 - using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;
- 10 enhancing correlation between residue centroid magnitude and residue solvent accessibility; and
 - defining the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment.
- 15 2. The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric.
- 20 3. The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.
- 25 4. The method of claim 1, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.
5. The method of claim 1, wherein the centroid of residue centroids represents a geometric center of the tertiary protein structure.

6. The method of claim 1, wherein the global linear hydrophobic moment characterizes an amphiphilicity of the tertiary protein structure.

5 7. The method of claim 1, wherein the global linear hydrophobic moment characterizes a magnitude of amphiphilicity of the tertiary protein structure.

8. The method of claim 1, wherein the global linear hydrophobic moment characterizes a direction of amphiphilicity of the tertiary protein structure.

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9. The method of claim 1, wherein the global linear hydrophobic moment is used to identify functional regions of the tertiary protein structure.

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10. A method for comparing at least two tertiary protein structures comprising a plurality of residues, for each tertiary protein structure, the method comprising the steps of:

calculating a centroid of residue centroids;
using the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

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enhancing correlation between residue centroid magnitude and residue solvent accessibility;

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defining the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment, the global linear hydrophobic moment characterizing an amphiphilicity of each tertiary protein structure; and

using the global linear hydrophobic moment of each tertiary protein structure to compare the amphiphilicity of the at least two tertiary protein structures.

11. The method of claim 10, wherein the centroid of residue centroids represents a geometric center of the tertiary protein structure.

5 12. The method of claim 10, wherein the global linear hydrophobic moment characterizes a magnitude and a direction of amphiphilicity of the at least two tertiary protein structures.

10 13. The method of claim 10, wherein the global linear hydrophobic moment is used to determine a hydrophobic imbalance arising from interaction of the at least two tertiary protein structures with each other.

14. An apparatus for calculating a moment of a tertiary protein structure comprising a plurality of residues, the apparatus comprising:

15 a memory; and
at least one processor operative to:
calculate a centroid of residue centroids;
use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

20 enhance correlation between residue centroid magnitude and residue solvent accessibility; and

define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment.

25 15. The apparatus of claim 14, wherein the centroid of the residue centroids represents a geometric center of the tertiary protein structure.

16. The apparatus of claim 14, wherein the global linear hydrophobic moment characterizes an amphiphilicity of the tertiary protein structure.

17. The apparatus of claim 14, wherein the global linear hydrophobic moment
5 is used to identify functional regions of the tertiary protein structure.

18. The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a distance metric.

10 19. The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using an ellipsoidal metric.

15 20. The apparatus of claim 14, wherein the correlation between residue centroid magnitude and residue solvent accessibility is enhanced using a solvent accessibility metric.

21. An article of manufacture for calculating a moment of a tertiary protein structure comprising a plurality of residues, comprising:

20 a computer-readable medium having computer-readable code embodied thereon, the computer-readable code comprising:

a step to calculate a centroid of residue centroids;

a step to use the centroid of residue centroids as a spatial origin of a global linear hydrophobic moment;

25 a step to enhance correlation between residue centroid magnitude and residue solvent accessibility; and

a step to define the global linear hydrophobic moment, wherein each of the residue centroids contributes a magnitude and direction to the global linear hydrophobic moment.